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Boundary bound states for the open Hubbard chain with boundary fields

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Abstract

The boundary effects in the open Hubbard chain with boundary fields are studied. The boundary string solutions of the Bethe ansatz equations that give rise to a wave functions localized at the boundary and exponentially decreasing away from the boundary are provided. In particular, it is shown that the correct ground state of the model at half-filling contains the boundary strings.

In view of the experimental possibilities [1], interest in the theoretical study of transport properties for one-dimensional electron systems has been considerably enhanced during recent years (see ref. [2] and references therein). Thus, theoretical investigations of Tomonaga-Luttinger liquids (see [3] and references therein) in the presence of boundaries and potential scatterers are of crucial importance. A conspicuous example of Tomonaga-Luttinger liquids with boundaries is provided by the one-dimensional Hubbard model with open boundaries and boundary fields (open Hubbard chain with boundary fields) [4, 5, 6, 7]. The Hamiltonian of this model is given by $H = H_{\rm bulk}^{\rm (open)} + H_{\rm boundary}$, where

$$H_{\rm bulk}^{\rm (open)} = -\sum_{j=1}^{L-1} \sum_{\sigma=\uparrow,\downarrow} (\psi_{j\sigma}^{\dagger}\psi_{j+1\sigma} + \psi_{j+1\sigma}^{\dagger}\psi_{j\sigma}) + U\sum_{j=1}^{L} n_{j\uparrow}n_{j\downarrow}, \tag{1}$$

$$H_{\rm boundary} = -h_1(n_{1\uparrow}+n_{1\downarrow}) - h_L(n_{L\uparrow}+n_{L\downarrow}). \tag{2}$$

Here U is the coupling constant, h_l is the boundary field at site $l \in \{1, L\}$, $\psi_{j\sigma}$ (resp. $\psi_{j\sigma}^{\dagger}$) denotes the annihilation (resp. the creation) operator of an electron with spin $\sigma \in \{\uparrow,\downarrow\}$ at site $j \in \{1, 2, \cdots, L\}$, and $n_{j\sigma} = \psi_{j\sigma}^{\dagger}\psi_{j\sigma}$ is the number operator. This model has been solved exactly by Bethe ansatz [4, 5, 6, 7], and its long-distance properties have been analyzed by using boundary conformal field theory [5, 6, 7]. Also, the boundary S matrices of the model have been obtained [8].

In this letter, focusing on the complex solutions of the Bethe ansatz equations, we proceed to study the boundary effects in the open Hubbard chain with boundary fields. Originally, such kind of work has been done in the case of open XXZ chain with boundary magnetic fields [9, 10]. In refs. [9, 10], the authors found *boundary string solutions* to the Bethe ansatz equations. The boundary strings represent *boundary bound states* which correspond to the wave functions localized at the boundaries. In particular, it was shown that, in the gapfull regime with appropriate conditions [11] on the boundary magnetic fields, the ground state contains the boundary 1-string.

We will show that, for the open Hubbard chain with boundary fields of type (2), there exist boundary bound states of the electrons corresponding to each boundary fields. If the boundary fields is sufficiently large ($h_l > 1$ for $l = 1, L$) then the rapidity configuration in the ground state of this model contains boundary strings.

Let us recall the Bethe ansatz solutions of the open Hubbard chain [4, 5, 6, 7]. The energy is represented as

$$E = -2\sum_{j=1}^{N} \cos k_j, \tag{3}$$

where the charge rapidities k_j are the solutions of the Bethe ansatz equations

$$e^{i2k_j(L+1)}\beta(k_j,h_1)\beta(k_j,h_L) = \prod_{\delta=1}^{M} e\left(2(\sin k_j - \Lambda_\delta)/c\right) e\left(2(\sin k_j + \Lambda_\delta)/c\right), \tag{4}$$

$$\prod_{\substack{\delta=1\\ \delta(\neq\gamma)}}^{M} e\left((\Lambda_\gamma - \Lambda_\delta)/c\right) e\left((\Lambda_\gamma + \Lambda_\delta)/c\right) = \prod_{j=1}^{N} e\left(2(\Lambda_\gamma - \sin k_j)/c\right) e\left(2(\Lambda_\gamma + \sin k_j)/c\right). \tag{5}$$

Here N and M respectively denote the number of electrons and electrons with down spin, and

$$c = U/2, \tag{6}$$

$$\beta(x,h) = \frac{1-he^{-ix}}{1-he^{ix}}, \tag{7}$$

$$e(x) = \frac{x+i}{x-i}. \tag{8}$$

Note that, in this model, the solutions of the Bethe ansatz equations are restricted as $\mathrm{Re}(k_j), \mathrm{Re}(\Lambda_\gamma) \geq 0$ and $k_j, \Lambda_\gamma \neq 0$.

Putting $k_{-j} = -k_j, \Lambda_{-\gamma} = -\Lambda_\gamma$ and $k_0 = 0, \Lambda_0 = 0$, we can rewrite the above Bethe ansatz equations into the more tractable forms,

$$e^{i2k_j(L+1)}\beta(k_j,h_1)\beta(k_j,h_L) = e\left(2\sin k_j/c\right)^{-1}\prod_{\delta=-M}^{M} e\left(2(\sin k_j - \Lambda_\delta)/c\right), \tag{9}$$

$$e\left(\Lambda_\gamma/c\right)^{-1}\prod_{\substack{\delta=-M\\ \delta(\neq\gamma)}}^{M} e\left((\Lambda_\gamma - \Lambda_\delta)/c\right) = \prod_{j=-N}^{N} e\left(2(\Lambda_\gamma - \sin k_j)/c\right). \tag{10}$$

Also, the energy is represented as

$$E = -\sum_{j=-N}^{N}\cos k_j + 1. \tag{11}$$

For the problems with periodic boundary conditions, we usually adopt the string hypothesis [12]. The string hypothesis states that, in the thermodynamic limit, the set of solutions $\{k_j, \Lambda_\gamma\}$ of the Bethe ansatz equations can be split into three kinds of solutions, which are real k_j's, combination of n Λ_γ's (Λ-strings of length n) and combination of n Λ_γ's and $2n$ k_j's (k-Λ-strings of length n) [12]. (We shall call these the *bulk* string solutions.) The Λ-strings and the k-Λ-strings can be interpreted as some kind of bound states [12, 13].

For the problems with open boundary conditions, since the equations (9) and (10) are very similar to the one for the model with periodic boundary conditions, it is reasonable to conjecture that the bulk strings make up the (sub)set of the solutions of the Bethe ansatz equations.

Boundary string

For the model with open boundary conditions, however, there may exist the complex solutions which are the different kind to the bulk strings. Note that, for the model with open boundary conditions, the energy (3) is the integrals of motion but the total momentum is not. Thus $\sum_{j=1}^{N} k_j$ does not have to be real, in contrast to the case of the periodic boundary conditions. The rapidity configurations which contain pure imaginary roots (or roots whose real parts are π) and do not contain the complex conjugate of these pure imaginary roots are admissible. (We shall call this kind of solutions which correspond to the boundary fields '*boundary string solutions*'. [9, 10])

One particle systems

As a warm-up exercise, we first consider the one electron system ($N = 1$). The wave function of the Bethe ansatz states is given by

$$\Phi_\sigma(n) \quad = A_\sigma(k)e^{ikn} - B_\sigma(k)e^{-ikn} \tag{12}$$

where $\sigma =\uparrow$ or $\downarrow$ is the spin of an electron. The relation between $A_\sigma(k)$ and $B_\sigma(k)$ is obtained by investigating the boundary scattering at left or right boundaries. The rapidity k is determined by the consistency condition for the left and right scatterings (Bethe ansatz equation). The boundary scattering at the boundary $n = 1$ gives

$$B_\sigma(k) = \frac{1 - h_1 e^{ik}}{1 - h_1 e^{-ik}} A_\sigma(k) \tag{13}$$

and at $n = L$ gives

$$B_\sigma(k) = \frac{1 - h_L e^{-ik}}{1 - h_L e^{ik}} e^{ik2(L+1)} A_\sigma(k). \tag{14}$$

The consistency condition for both left and right scatterings gives

$$\frac{1 - h_1 e^{ik}}{1 - h_1 e^{-ik}} \frac{1 - h_L e^{ik}}{1 - h_L e^{-ik}} = e^{2ik(L+1)}. \tag{15}$$

There are two type of solutions for (15): one is the real solution which correspond to the free particle interacting at the boundary, the other is the pure imaginary solution which can be interpreted as the bound state at the boundary. When k is pure imaginary, the right hand side of (15) decreases exponentially fast in the thermodynamic limit (we deal with only the case $\mathrm{Im}(k) > 0$). Therefore, if eq. (15) has pure imaginary solution, the rapidity k must take values of which the left hand side of (15) vanishes. Let $k_{(1)} = i\chi_{(1)}, k_{(L)} = i\chi_{(L)}$ be the pure imaginary solutions such as

$$\begin{aligned} 1 - e^{-\chi_{(1)}} h_1 &\sim e^{-2\chi_{(1)}(L+1)}, \\ 1 - e^{-\chi_{(L)}} h_L &\sim e^{-2\chi_{(L)}(L+1)}. \end{aligned} \tag{16}$$

Note that the above equations have solution with $\chi_{(l)} > 0$ only when $h_l > 1$ ($l = 1, L$). The solution $k_{(1)}$ ($k_{(L)}$) corresponds to the wavefunction localized at the site 1: $\Phi_\sigma \sim e^{-n\chi_{(1)}}$ (resp. site L: $\Phi_\sigma \sim e^{-(L-n)\chi_{(L)}}$)

Ground state

Now we investigate the ground state of the open Hubbard chain with boundary fields at the half filling[1]. For the model with periodic boundary conditions, in the ground state, the rapidities $\{k_j, \Lambda_\gamma\}$ are all real and fill the Fermi seas. However, as examined above, we must consider the possibility of the existence of the boundary strings. Our task is, then, to compare the energy of the configuration with boundary strings to that of the configuration without the boundary strings. (In the remainder

[1]In this letter, the term half-filling means that the real charge rapidities k_j fill the Fermi-sea between $-\pi$ and π.

of this letter, we treat only the case that the real roots $\{k_j, \Lambda_\gamma\}$ fill the Fermi-seas.) To calculate the effect of the existence of the boundary strings to the energy, we must investigate, in addition to the energy of the boundary strings, the shift of the densities of the real roots due to the existence of the boundary strings.

We shall introduce the densities of roots and holes. The number of allowed solutions for the Bethe ansatz equations (4) and (5) in the intervals $(k,\, k+dk)$ and $(\Lambda,\, \Lambda+d\Lambda)$ are expressed as $L[\rho(k)+\rho^h(k)]dk$ and $L[\sigma(\Lambda)+\sigma^h(\Lambda)]d\Lambda$. Here $\rho(k)$ and $\sigma(\Lambda)$ are the densities of roots (filled solutions), and $\rho^h(k)$ and $\sigma^h(\Lambda)$ are the densities of holes (unfilled solutions).

If there exist two boundary strings $\chi_{(1)} = \ln h_1$, $\chi_{(L)} = \ln h_L$ for each boundary fields (and there do not exist holes in the real roots), the densities $\rho(k)$, $\sigma(\Lambda)$ satisfy the following integral equations

$$\begin{aligned}
\rho(k) &= \frac{1}{\pi} + 2\cos k \int_{-B}^{B} d\Lambda \sigma(\Lambda) K(2(\sin k - \Lambda)) \\
&\quad + \frac{1}{L}\left[\frac{1}{2\pi}(\xi(k,h_1)+\xi(k,h_L)) - 2\cos k K(2\sin k)\right], \qquad (17) \\
\sigma(\Lambda) &= 2\int_{-Q}^{Q} dk \rho(k) K(2\Lambda - 2\sin k) - \int_{-B}^{B} d\Lambda' \sigma(\Lambda') K(\Lambda-\Lambda') \\
&\quad + \frac{1}{L}\left[\frac{2c}{c-2\sinh\chi_{(1)}} K(\frac{2c\Lambda}{c-2\sinh\chi_{(1)}}) + \frac{2c}{c+2\sinh\chi_{(1)}} K(\frac{2c\Lambda}{c+2\sinh\chi_{(1)}})\right] \\
&\quad + \frac{1}{L}\left[\frac{2c}{c-2\sinh\chi_{(L)}} K(\frac{2c\Lambda}{c-2\sinh\chi_{(L)}}) + \frac{2c}{c+2\sinh\chi_{(L)}} K(\frac{2c\Lambda}{c+2\sinh\chi_{(L)}})\right] \\
&\quad - \frac{1}{L} K(\Lambda), \qquad (18)
\end{aligned}$$

where $\xi(k,h) = (h^2-1)/(1-2h\cos k + h^2)$, $K(x) = c/[\pi(x^2+c^2)]$. Here Q and B are charge and spin pseudo Fermi-momentum, respectively. We assume that, to examine the densities of order $O(1/L)$ in the half filled case, we can take $B=\pi$ and $Q=\infty$.

If we separate the densities into the part of order $O(L^0)$ and $O(1/L)$ as

$$\begin{aligned}
\rho(k) &= \rho_0(k) + \frac{1}{L}\rho_1(k) + O(\frac{1}{L^2}) \\
\sigma(\Lambda) &= \sigma_0(\Lambda) + \frac{1}{L}\sigma_1(\Lambda) + O(\frac{1}{L^2}), \qquad (19)
\end{aligned}$$

then $\rho_0(k)$ and $\sigma_0(\Lambda)$ are identical to the densities of k's and Λ's, respectively, for the ground state with periodic boundary conditions. The ground state energy of the model with periodic boundary conditions is, then, given by

$$E_{\mathrm{periodic}} = -L\int_{-\pi}^{\pi} dk \rho_0(k)\cos k. \qquad (20)$$

The $O(1/L)$ contribution $\rho_1(k)$ can be divided into three parts which reflect the geometry (open boundary conditions), the effect of the boundary fields, and the existence of the boundary strings;

$$\rho_1(k) = \rho_{\mathrm{geom}}(k) + \rho_{\mathrm{field}}(k) + \rho_{\mathrm{string}}(k). \qquad (21)$$

We further separate $\rho_{\rm field}(k)$ to $\rho_{\rm field}(k) = \rho_{\rm field}(k, h_1) + \rho_{\rm field}(k, h_L)$ where $\rho_{\rm field}(k, h_l)$ is the contribution from the boundary field h_l, and $\rho_{\rm str}(k)$ to $\rho_{\rm str}(k) = \rho_{\rm str}(k, h_1) + \rho_{\rm str}(k, h_L)$ where $\rho_{\rm str}(k, h_l)$ is the contribution from the boundary string corresponding to the boundary field h_l.

Here $\rho_{\rm geom}(k)$ is given by

$$\rho_{\rm geom}(k) = -\frac{\cos k}{2\pi}\int_{-\infty}^{\infty} dw \frac{e^{-iw\sin k - c|w|/2}}{1+e^{c|w|}} - 2\cos k K(2\sin k), \tag{22}$$

and $\rho_{\rm field}(k, h)$ is given by

$$\rho_{\rm field}(k, h) = \frac{\xi(k, h)}{2\pi} - \frac{\cos k}{2\pi^2}\int_{-\pi}^{\pi} dk' \int_{-\infty}^{\infty} dw \frac{e^{-2iw(\sin k - \sin k') - c|w|}}{\cosh(cw)}. \tag{23}$$

The form of $\rho_{\rm str}(k, h)$ is depend on the value of the boundary field h.

The energy in the case that there are boundary strings, is given by

$$E = -L\int_{-\pi}^{\pi} dk \rho_0(k)\cos k - \int_{-\pi}^{\pi} dk \rho_1(k)\cos k - 2(\cosh\chi_1 + \cosh\chi_L). \tag{24}$$

Then the energy difference between the configuration which contains boundary string and the configuration which does not contain the boundary string, corresponding to the boundary field h_l, is given by

$$\Delta E(h_l) = -2\cosh\chi_l + e(h_l), \tag{25}$$

where

$$e(h_l) = -\int_{-\pi}^{\pi} dk \rho_{\rm str}(k, h_l)\cos k. \tag{26}$$

If the strength of the boundary field h_l is such that $c < |2\sinh\chi_l|$, then

$$\rho_{\rm str}(k, h_l) = 4c\cos k\int_{-\infty}^{\infty} d\Lambda \frac{K\left(\frac{2c\Lambda}{2\sinh\chi_l - c}\right)K(2\sin k - 2\Lambda)}{2\sinh\chi_l - c}, \tag{27}$$

and

$$e(h_l) = -\frac{1}{L}\int_{-\pi}^{\pi} dk \int_{-\infty}^{\infty} d\Lambda \frac{4c\cos^2 k}{2\sinh\chi_l - c} K\left(\frac{2c\Lambda}{2\sinh\chi_l - c}\right)K(2\sin k - 2\Lambda). \tag{28}$$

Noticing $K(x) > 0$ (x is real), we see that $e(h_l) < 0$.

On the other hand, if $|2\sinh\chi_l| < c$, then

$$\rho_{\rm str}(k, h_l) = \frac{\cos k}{4\pi}\left[G\left(\frac{c}{2} - \sinh\chi_l, k\right) + G\left(\frac{c}{2} + \sinh\chi_l, k\right)\right], \tag{29}$$

where

$$G(x, y) = \int_{-\infty}^{\infty} dw \frac{e^{-iw\sin y - x|w|}}{\cosh cw/2} = \frac{x}{2\pi}\int_{-\infty}^{\infty} d\Lambda \frac{K(c(\Lambda - \sin y)/x)}{\cosh(\pi\Lambda/c)}. \tag{30}$$

In this case, $e(h_l)$ is given by

$$e(h_l) = -\frac{1}{L}\int_{-\pi}^{\pi} dk \frac{\cos^2 k}{4\pi}\left[G(\frac{c}{2} - \sinh\chi_l, k) + G(\frac{c}{2} + \sinh\chi_l, k)\right]. \quad (31)$$

Again, noticing $G(x, y) > 0$ $(x > 0)$, we see that $e(h_l) < 0$.

We thus conclude that the configuration which contains boundary strings has lower energy than the configuration which does not contain the boundary strings. Therefore, if $h_l > 1$ for $l = 1, L$, the ground state rapidity configuration of the open Hubbard chain with boundary fields at the half-filling contains the boundary strings for each boundary fields.

The surface energy of the Hubbard chain with boundary fields

$$E_{\text{surface}} = E^{\text{gr}} - E^{\text{gr}}_{\text{periodic}}, \quad (32)$$

where E^{gr} is the ground state energy of the Hamiltonian H and $E^{\text{gr}}_{\text{periodic}}$ is the ground state energy of the model with periodic boundary conditions, is given by

$$E_{\text{surface}} = -\int_{-\infty}^{\infty} dk[\rho_{\text{geom}}(k) + \rho_{\text{field}}(k) + \rho_{\text{str}}(k)]\cos k \\ -2(\cosh\chi_1 + \cosh\chi_L). \quad (33)$$

Conclusion

Although, we did not yet performed to classify the all solutions of the Bethe ansatz equations (4) and (5), we have found that there exist the boundary string solutions in addition to the bulk strings.

It was known that the open Hubbard chain with another type of the boundary fields $H'_{\text{boundary}} = -h_1(n_{1\uparrow} - n_{1\downarrow}) - h_L(n_{L\uparrow} - n_{L\downarrow})$ can be solved. The related Bethe ansatz equations for this Hamiltonian contain factors which depend both the coupling constant and boundary fields [6, 7]. The analysis of these Bethe ansatz equations will be appeared elsewhere.

After this letter was written up, we find the preprint which relates to our results [14]. In their paper, boundary strings for the both charge and spin rapidities are studied.

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